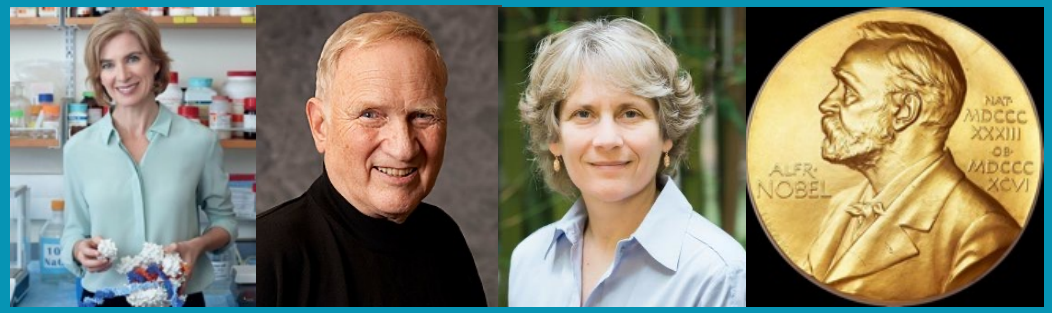
Remarks to the NERSC User Group
Director Mike Witherell
Oct. 12, 2022
BERKELEY LAB
U.S. DEPARTMENT OF
ENERGY

What does the Nation Need from Berkeley Lab?



ALS ADVANCED LIGHT SOURCE

NERSC

ESnet ENERGY SCIENCES NETWORK

JBEI

BERKELEY LAB MOLECULAR FOUNDRY

JGI JOINT GENOME INSTITUTE

- Scientific solutions addressing national priorities: Energy and climate, resilience, the environment, health, security, and the economy
- Discovery Science
- Unique scientific capabilities and facilities
  - National user facilities
  - Advanced instrumentation
- Managed, large research teams, including many deep collaborations with other DOE Labs
- Important technologies of strategic national interest with long, difficult R&D paths
- Response to national emergencies
- A diverse group of highly trained, creative individuals committed to working together in teams on these grand national challenges

Research Areas and Leadership

Carol Burns
Dep. Director for Research & CRO

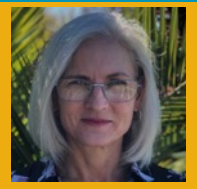
Michael Witherell
Lab Director

Michael Brandt
Dep. Director for Ops & COO

CTO

Chief DEI Officer

CRO Senior Advisor



Chief of Staff

Deputy COO

Chief Financial Officer

Chief Comms Officer

Chief Counsel

Chief Eng. Officer

BIOSCIENCES
Paul Adams, ALD

COMPUTING SCIENCES
Jonathan Carter, ALD

EARTH & ENVIRO. SCIENCES
Jens Birkholzer, ALD

ENERGY SCIENCES
Jeff Neaton, ALD

ENERGY TECHNOLOGIES
Ravi Prasher, ALD

PHYSICAL SCIENCES
Natalie Roe, ALD

Our User Facilities have national impact.

The user facilities are collaboration centers, providing the tools and the expertise needed by a diverse research community to address the grand national challenges.

Bright x-ray beams and leading instruments for chemistry, materials, biology, and more. FY21 Users: 1,149

HPC for all DOE science: simulation, data analytics, and machine learning. FY21 Users: 9,183

Integrative and collaborative genome science FY21 Users: 2,180

Expertise and instruments for nanoscale science, QIS, and electron microscopy FY21 Users: 1,670

The leading research network connecting DOE labs and experiments. 1,140 Peta-bytes/yr. in FY21

BERKELEY LAB

U.S. DEPARTMENT OF ENERGY

Strategic Priorities to Shape the Future of the Laboratory

CHEMISTRY and MATERIALS SCIENCE with the ALS and Molecular Foundry

COMPUTING SCIENCES ENABLING SCIENTIFIC DISCOVERY

NEW CAPABILITIES in BIOLOGICAL and ENVIRONMENTAL SCIENCE

DISCOVERY SCIENCE in FUNDAMENTAL PHYSICS

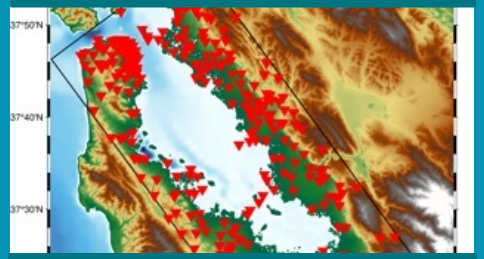
ATTRACT, RECRUIT and RETAIN THE DIVERSE WORKFORCE OF THE FUTURE

INFRASTRUCTURE RENEWAL

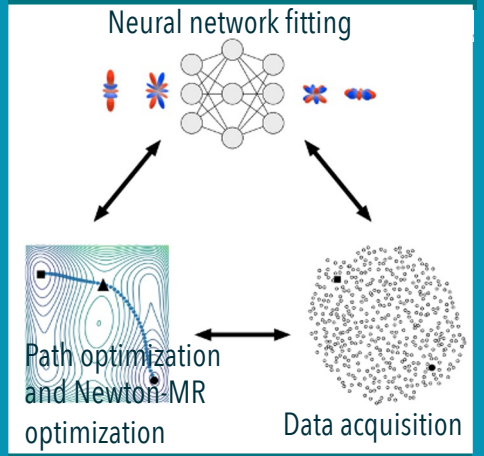
ACCELERATING DECARBONIZATION: A strategic priority that draws on all of the capabilities across the Laboratory

We use LDRD to develop new capabilities.
This year we selected three multi-area approaches to accelerating discovery.

Machine Learning



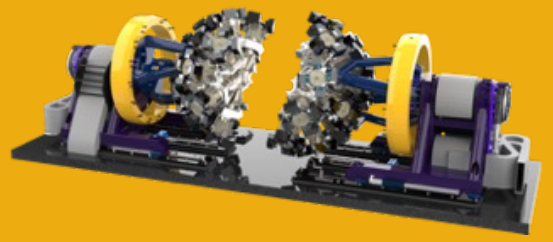
AI-enabled earthquake simulation

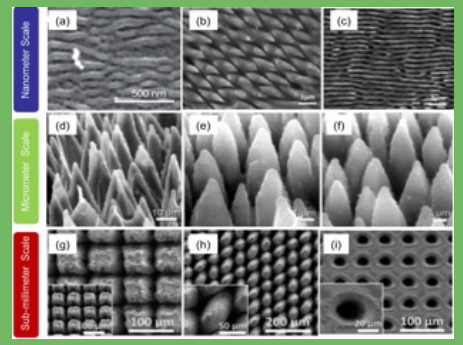


ML for chemistry and energy technologies

Lab Automation

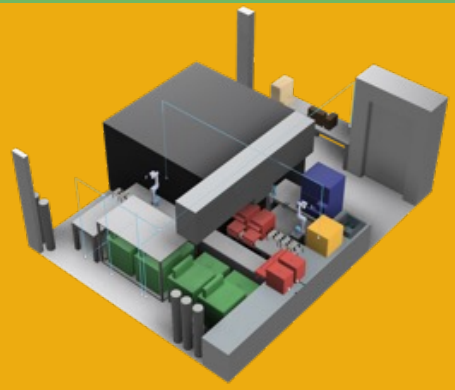
Real-time processing of NP/HEP data





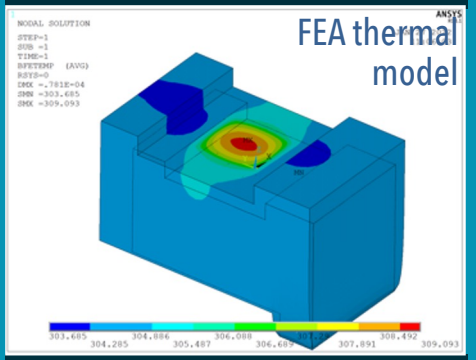
Self-driving materials discovery

Self-guiding field labs

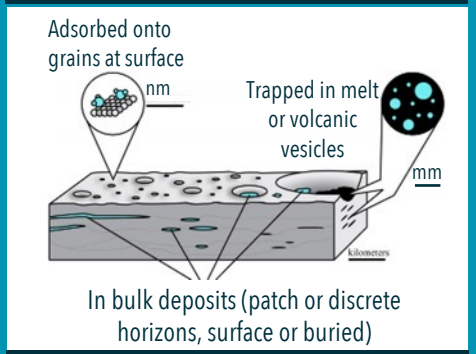


Closed-loop materials synthesis

Advanced Instrumentation



Optimized crystallography beamlines @ ALS



Lunar geoscience with ALS

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Accelerating Scientific Discovery Through AI, Applied Math and Data

Interdisciplinary teams of domain scientists working with Computing/Data researchers throughout the Lab

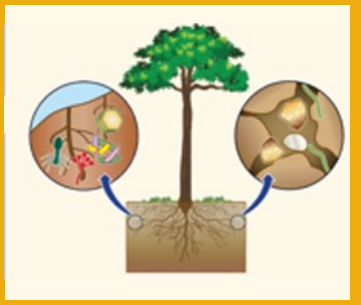
Impact Across SC includes User Facilities and Large-Scale Experiments

Fabricated Ecosystems

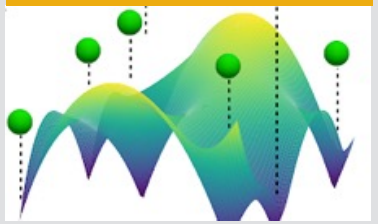
Telescopes and Colliders

Light Sources

Environ-mental Sensors



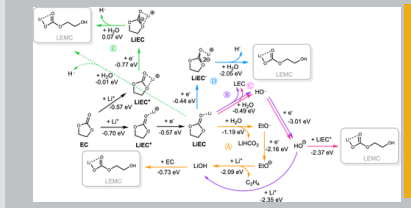
Mathematics



CAMERA; Techniques and Algorithms

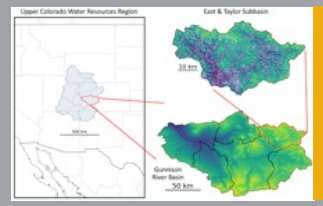
Automation

Self-driving labs; Instrument control and tuning



Optimizing Materials Design

Design for function; Optimized synthesis



Surrogates and Data-driven models

Faster execution; Multi-scale

Data Resources

JGI JOINT GENOME INSTITUTE

PDG particle data group

KBase

ESS-DIVE Deep Insight for Earth Science Data

NEURODATA WITHOUT BORDERS

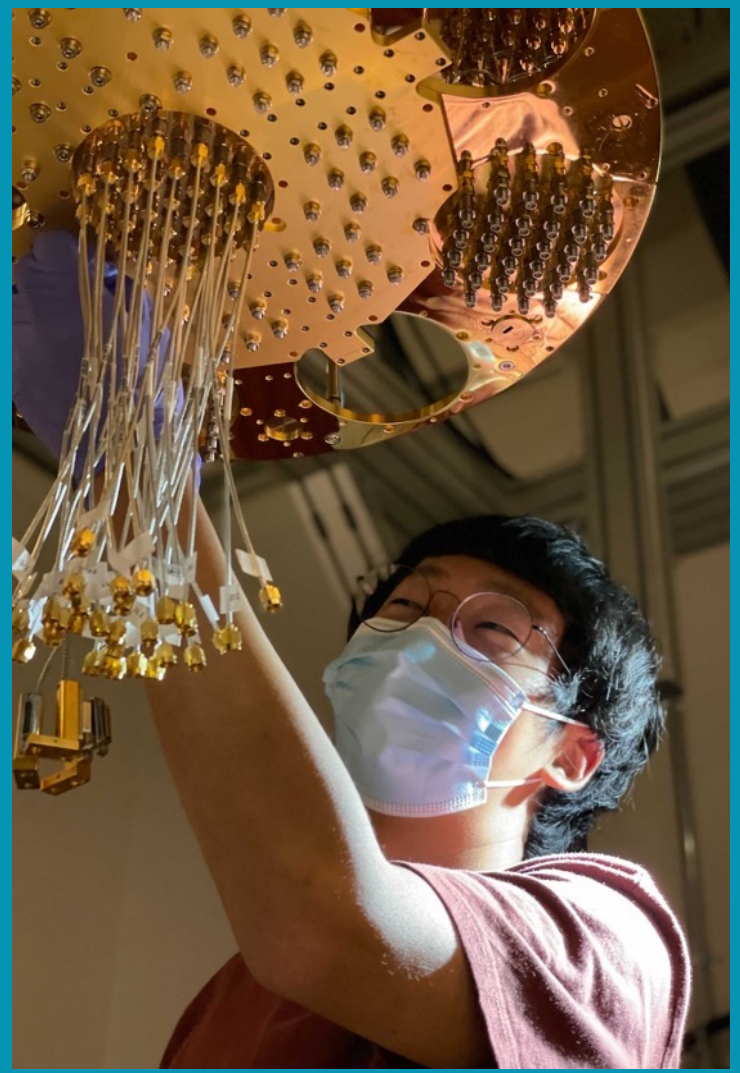
AMERIFLUX MANAGEMENT PROJECT

nmdc National Microbiome Data Collaborative

MATERIALS PROJECT

NGEE–TROPICS NEXT-GENERATION ECOSYSTEM EXPERIMENTS

Quantum Information Science and Technology



This lab-wide emerging capability enables fundamental advances for all SC Program Offices:

QUANTUM SYSTEMS ACCELERATOR
Catalyzing the Quantum Ecosystem

- **Quantum Hardware**
  - Advanced Quantum Testbed
  - AI-enabled Control for Enhancing Quantum Transduction
- **Quantum Materials**
  - Quantum Coherence EFRC
  - Molecular Foundry QIS
  - Quantum Materials Program
  - ALS Quantum Materials Research & Discovery
  - Superconducting Structures
- **Quantum Communications and Networks**
  - QUANT-NET
- **Quantum Software and Protocols**
  - Advancing Integrated Development Environments for Quantum Computing
  - NERSC QIS Program
  - Berkeley Quantum Synthesis Toolkit
- **Advancing Science with Quantum**
  - QuantISED Quest Program for HEP
  - Adiabatic Quantum Computing for NP
  - Qubit synthesis far from equilibrium FES
  - Earth Quantum Lab
- **Training the Quantum Workforce**
  - QIS Internships
  - QuantumCAMP

Thank you to NERSC Users

Jean Sexton

… instrumental in debugging UVM (Unified Virtual Memory) issues during the Perlmutter Phase 1 deployment, and during the integration of Phase 2

Derek Mendez

… instrumental in debugging mpi4py issues, helping to prepare Perlmutter for many data-oriented HPC workloads

Noel Keen

… instrumental in debugging network issues during the integration of Perlmutter Phase 2, and in early of testing Phase 2.

Thank You